

Finite size scaling with modified boundary conditions

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An efficient scheme is introduced for a fast and smooth convergence to the thermodynamic limit with finite size cluster calculations. This is obtained by modifying the energy levels of the non interacting Hamiltonian in a way consistent with the corresponding one particle density of states in the thermodynamic limit. After this modification exact free electron energies are obtained with finite size calculations and for particular fillings that satisfy the so called "closed shell condition". In this case the "sign problem" is particularly mild in the auxiliary field quantum Monte Carlo technique and therefore, with this technique, it is possible to obtain converged energies for the Hubbard model even for $U > 0$. We provide a strong numerical evidence that phase separation occurs in the low doping region and moderate $U \lesssim 4t$ regime of this model.

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After several years of scientific effort, based on advanced analytical and numerical methods, only very few properties of the 2D Hubbard model have been settled. The 2D Hubbard model is defined in a square lattice containing a finite number L (N_h) of sites (holes):

$$H = K + V = -t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_i^\uparrow n_i^\downarrow \quad (1)$$

with standard notations, the kinetic energy operator K being equal to H for $U = 0$. In the thermodynamic limit, namely for $L \rightarrow \infty$ at given doping $\delta = N_h/L$ fundamental issues such as the existence of a ferromagnetic phase at large U/t ratio and/or the stability of an homogeneous ground state with possible d-wave superconducting properties are still highly debated, as several approximate numerical techniques lead to controversial and often conflicting results. This situation is particularly important right now, since recent progress in the realization of fermionic optical lattices could lead to the experimental realization of the fermionic Hubbard model.

Method: We consider the square lattice and generic finite clusters that satisfy all the symmetries of the infinite system. As well known finite square lattices can be defined by two integers n, m such that $n^2 + m^2 = L$, obtained by supercell translation vectors $\tau_x = (n, m)$ and $\tau_y = (-m, n)$. In order to fulfill rotation symmetries, two sequences can be defined:

$$\begin{aligned} m = 0 \quad L = n \times n \quad &\text{The usual sequence} \\ m = n \quad L = 2n^2 \quad &\text{The } 45^\circ \text{ degrees tilted sequence} \end{aligned} \quad (2)$$

On the other hand translation symmetries are recovered by employing periodic or antiperiodic boundary conditions, the same in both directions τ_x and τ_y in order to preserve rotation and reflection symmetries.

In the following we would like to consider the most useful sequence of clusters for converging as fast as possible to the thermodynamic limit. A simple technique,

well known in strongly correlated lattice models¹ and in realistic calculations² is to consider the twisted averaged boundary conditions (TABC) method. This technique allows an exact evaluation of converged thermodynamic quantities (energy, density matrix, etc.) in the non interacting $U = 0$ limit.¹ Indeed it has been proven very successful to reduce substantially the finite size effects in several correlated systems.

In the following we follow a different approach analogous to TABC in the requirement to remove finite size effects in the non interacting limit. However the proposed approach can be used more efficiently in combination with the auxiliary field quantum Monte Carlo (AFQMC) method.^{3,4} The latter technique is one of the most powerful ones used so far for the study of the Hubbard model, as it can project out from a mean-field (Slater determinant) state $|MF\rangle$, the exact ground state of the Hamiltonian by the application of the imaginary time propagation $\exp(-\tau H)$, for large τ . Here we consider variational expectation values (Var) on the $\exp(-\tau/2H)|MF\rangle$ state and non variational mixed estimators (no Var) between the previous state and $\exp(-\tau/2H)|\psi_0\rangle$, $|\psi_0\rangle$ being the ground state Slater determinant for $U = 0$. Both quantities clearly converge to exact values for large τ ⁵.

The sign problem occurs at finite doping and $U/t > 0$ but it is particularly mild when i) the $U = 0$ Hamiltonian has a non degenerate ground state, a situation that occurs for particular fillings- the closed shell fillings- in any finite clusters, ii) the auxiliary field transformation is real, as with the proposed approach it is not necessary to sample a complex phase. Until now several reliable and "numerically exact" calculations have been performed by means of this technique on moderately large clusters (i.e. up to $\simeq 100$ sites and $U/t \lesssim 4t$)⁶⁻⁹ but it was difficult to establish thermodynamically converged results, especially in the weakly correlated regime. One should also mention that, recently, a remarkable progress has been made, allowing the complete removal of the time dis-

cretization error in the propagator^{6,10,11}, a development that will not be used here, as we have preferred to use a small enough time step $\Delta\tau$, such that this systematic error is negligible, at least as far as the ground state energy is concerned.

Let us now introduce the method. Consider a finite cluster. The kinetic energy can be written in Fourier space, by collecting k points related by point symmetries to the same energy shell ϵ_i :

$$K = \sum_{i,\sigma} \epsilon_i \sum_{k_i | \epsilon_k = \epsilon_i} c_{k,\sigma}^\dagger c_{k,\sigma} \quad (3)$$

where $\epsilon_k = -2t(\cos k_x + \cos k_y)$ in 2D. We can assume that the energy levels ϵ_i are defined in ascending order. Each shell occurs with some multiplicity g_i and:

$$L = \sum_{i=1}^p g_i \quad (4)$$

where p is the number of different energy levels. In the square lattice case we can choose for simplicity clusters that do not contain accidental degeneracies ($g_i \leq 8$), namely they are given by the second sequence given in Eq.(2) with PBC (APBC) for n odd (even). The fundamental quantity that we are going to use in order to achieve more easily the thermodynamic limit is the density of states $N(E)$:

$$N(E) = \int \frac{dk^d}{(2\pi)^d} \delta(E - \epsilon_k) \quad (5)$$

defined in a way that $\int N(E)dE = 1$. This function can be evaluated analytically and/or computed with arbitrary accuracy in the thermodynamic limit for any given lattice model. We partition the energy bandwidth of the lattice (e.g. $-4t < E < 4t$ in the square lattice) in intervals $\bar{\epsilon}_i$ such that:

$$g_i/L = \int_{\bar{\epsilon}_{i-1}}^{\bar{\epsilon}_i} N(E)dE \quad (6)$$

The above equation define all the levels $\bar{\epsilon}_i$ by simple induction, because once we know, e.g. $\bar{\epsilon}_n$ we can solve the above equation for $i = n + 1$ and we can obtain univocally $\bar{\epsilon}_{n+1}$. Therefore by setting $\bar{\epsilon}_0$ equal to the lowest one electron energy ($-4t$ in the 2D square lattice), all levels $\bar{\epsilon}_i$ can be computed and their level spacing is in exact correspondence with the density of states. Notice that for the particular symmetry of the DOS in bipartite lattices $N(E) = N(-E)$, due to particle-hole symmetry, it follows that one of the levels is exactly vanishing.

After the above decomposition, in order to fulfill the requirement to have an exact energy for $U = 0$ we can modify the energy levels of the kinetic energy $\epsilon_i \rightarrow \tilde{\epsilon}_i$ in

the following way:

$$\tilde{\epsilon}_i = \frac{\int_{\bar{\epsilon}_{i-1}}^{\bar{\epsilon}_i} EN(E)dE}{\int_{\bar{\epsilon}_{i-1}}^{\bar{\epsilon}_i} N(E)dE} = L/g_i \int_{\bar{\epsilon}_{i-1}}^{\bar{\epsilon}_i} EN(E)dE \quad (7)$$

where the latter equality comes just from the definition in Eq.(6). In this way the revised kinetic energy $K \rightarrow \bar{K}$ is obtained by replacing ϵ_i with $\tilde{\epsilon}_i$ in Eq.(3). It is immediate to show that, when we satisfy the closed shell condition, i.e. $N = \sum_{i \leq i_F} g_i$, within these modified boundary conditions (MBC) we obtain straightforwardly that the ground state energy per site is:

$$< K/L > = 2 \sum_{i \leq i_F} \frac{g_i}{L} \tilde{\epsilon}_i = 2 \int_{\bar{\epsilon}_0}^{\bar{\epsilon}_{i_F}} EN(E)dE \quad (8)$$

namely the exact energy per site for $U = 0$ at the thermodynamic density:

$$N/L = 2 \int_{\bar{\epsilon}_0}^{\bar{\epsilon}_{i_F}} N(E)dE$$

, where the factor two in the above equation takes into account the spin components.

At finite U it is quite simple to show that the above sequence of lattices with MBC converges to the exact thermodynamic limit because for large L the modification of the levels, as compared to the original ones, becomes irrelevant.

In this way we have several advantages and simplifications:

- The Hamiltonian is always real with MBC (a positive property for the sign problem).¹²
- The non interacting exact limit is obtained for the closed shell fillings. Thus we expect less size effects just for those particular densities less affected by the sign problem within AFQMC.
- The MBC satisfy all the symmetries of the infinite systems. For instance when we apply TABC, each boundary with a non zero twist generally breaks all point spatial group symmetries, maintaining only translation symmetry. This may not affect the average result, but it becomes certainly more difficult to converge to the exact result, i.e. one needs larger projection times in AFQMC due to smaller finite size gaps that occur after a small symmetry breaking perturbation of the Hamiltonian given by a tiny twist of the boundary conditions.
- Last but not least, MBC are rather trivial to implement in the AFQMC as it is enough to change the propagator $\exp(-\Delta\tau K) \rightarrow \exp(-\Delta\tau \bar{K})$. This

matrix is never sparse and has to be computed in advance within AFQMC for its efficient implementation. Thus the use of MBC does not lead to any overhead in the performances of the algorithm.

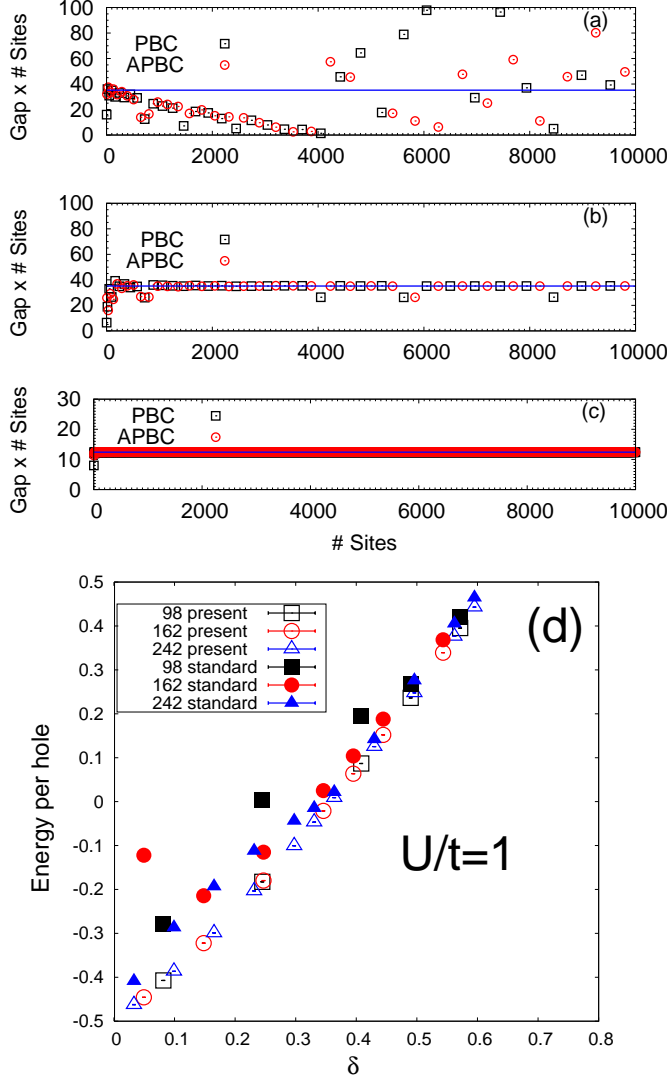


FIG. 1: $U = 0$ energy gap for finite clusters with non degenerate ground state at the closest filling $N/L = 0.9$ with 45° tilted PBC or APBC. This gap is multiplied by the number sites, as it should converge for $L \rightarrow \infty$ to $g/N(\mu)$, where μ is the thermodynamic chemical potential at this filling and g is the multiplicity of the energy level ($g = 8$ in 2D and $g = 2$ in 1D). (a): standard 2D clusters. (b) modified 2D clusters according to this work (see text). (c): standard 1d clusters. (d) Energy per hole for standard clusters with PBC (filled symbols) and with MBC (empty symbols).

As it is shown in Fig.(1a-c), the most important problem in the usual sequence of finite clusters is that the $U = 0$ finite size gap behaves erratically when L increases, in spatial dimensionalities $D > 1$ and away from commensurate fillings. This precludes to obtain accurate

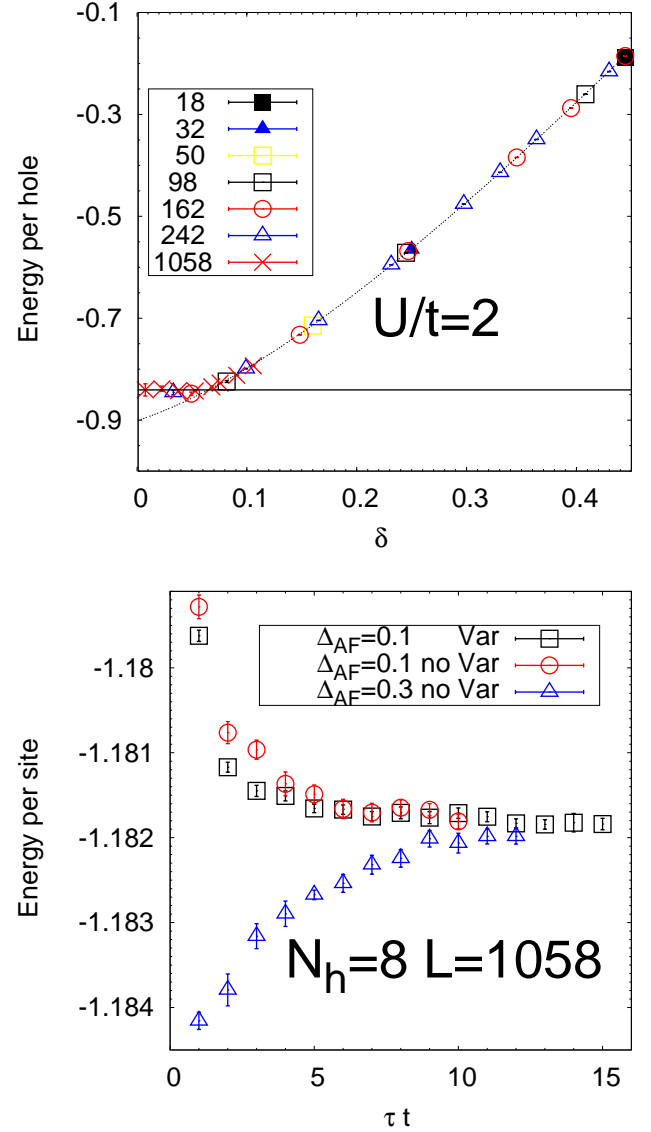


FIG. 2: Upper panel: Energy per hole in the 2D Hubbard model. Finite size effects are rather well behaved by using MBC and at small doping the energy per hole approaches almost exactly an horizontal line. This implies phase separation as discussed in the text. The dashed line is a fit (see table) of the data for $\delta > 6.5\%$. Lower panel: energy vs τ convergence starting with several initial left and right wave functions. "Var" ("no Var") stands for the (non-)variational calculation (see text) with different values of the antiferromagnetic parameter Δ_{AF} in the mean-field determinant.

extrapolations to the thermodynamic limit at least for moderate U/t and finite dopings (see e.g. Fig.1d). As it is evident in Fig.(1a-b) the MBC behave much better in this respect. Only few clusters scatter from the converged $\simeq g/N(E)$ energy level separations, but they correspond to atypical lattices when $g_i \neq 8$ at the highest occupied or lowest unoccupied free-electron energy

levels. Remarkably a reasonably converged value of this quantity occurs only after few hundreds sites, which is feasible for a numerical approach (see e.g. Fig. 1d).

Results: we have carried out a systematic finite size scaling study of the energy per hole in the moderate U/t regime. As pointed out in the milestone paper by Emery and Kivelson¹³ a minimum at doping δ_c in the energy per hole, corresponding to a given variational ansatz, implies its instability against phase separation because it is possible to gain energy for $\delta \leq \delta_c$ by segregating the holes in a hole rich region with the same type of ansatz. In an exact calculation, whenever it is possible to carry out the thermodynamic limit, clearly we have to obtain a constant energy per hole in all the region $\delta \leq \delta_c$, just because the compressibility - e.g. the slope in the energy per hole at $\delta \rightarrow 0$ -, cannot be negative in an exact calculation. As shown in Fig. 2(a), at $U/t = 2$ we can safely reach the thermodynamic limit with the clusters considered, thanks to the very small finite size effects introduced by the method proposed in the previous section, that, in this case, look considerably smaller than standard TABC⁸. The convergence in imaginary time is quite clear also for the most difficult case at small doping (see Fig. 2b) and also independent of the initial trial function used. In this case we have used a mean field state with a non zero antiferromagnetic order parameter Δ_{AF} along the x - spin direction.⁶ In the more difficult cases for larger U/t we have also used a d-wave order parameter $\Delta_{x^2-y^2}^{BCS}$ in order to converge faster or at least for obtaining the lowest possible variational energies compatible with a reasonable average sign $\langle s \rangle \geq 0.05$. It is clear that this by no means implies the existence of a non zero superconducting order parameter in the ground state, an issue that will not be discussed in the present work.

At $U/t = 2$ the achieved flat behavior of the energy

per hole for $\delta \leq 6.5\%$ clearly indicates the accuracy of the AFQMC at this small coupling, that is indeed able to determine phase separation just by imaginary time projection of an homogeneous trial state. At larger coupling (see Ref.14), though we have not been able to reach the same cluster size and the same length of the projection times, the accuracy in the energy per hole appears acceptable and allow us to determine the phase separated region for $U \leq 4t$ (see table). Notice that, in this table, the energy gain to have phase separation can be measured by the difference of the minimum hole energy E_{min}^h obtained for the largest clusters at doping $\delta \leq \delta_c$ and the hole energy a_0 extrapolated at $\delta = 0$ using only doping values clearly outside the phase separated region. In other words a_0 represents the energy per hole of the uniform phase extrapolated at zero doping. This difference $a_0 - E_{min}^h$ appears to be very large $\simeq 0.1t$ at $U/t = 2, 3$ and less evident for $U/t = 4$. This is probably the reason why at $U/t = 4$, there have been several controversial claims^{6,8,9,15}. Given this behavior, it is also possible that, at larger U/t , the phase separation may be less evident and δ_c may significantly decrease¹⁶, despite some works indicate exactly the opposite effect^{8,17}. It is clear that at large U/t this important issue remains still open. On the other hand, at $U/t = 1$, we have not obtained evidence of phase separation, because probably we cannot reach enough small doping values with the affordable finite clusters $L \lesssim 1058$. Indeed at this coupling value also the antiferromagnetic order parameter m_{AF} cannot be detected numerically, being extremely small even at $\delta = 0$. Since the existence of antiferromagnetism is at the basis of the phase separation argument¹³ it is possible that also δ_c can be exponentially small at small U/t , as is the case for $m_{AF} \simeq \exp(-\propto 1/\sqrt{t/U})$ within the Hartree-Fock theory³.

U/t	E_{min}^h	δ_c	a_0	a_1	a_2	a_3	a_4	a_5	Δ_{max}
1	-0.484(13)	0.00(1)	-0.49185	0.88825	1.99156	-2.46827	2.20290	-0.73928	0.00053
2	-0.843(1)	0.067(5)	-0.90164	0.73469	3.45846	-4.87765	4.03989	-1.27852	0.00062
3	-1.125(1)	0.105(10)	1.20909	0.41515	4.84506	-6.43761	4.74676	-1.35904	0.00034
4	-1.342(2)	0.110(15)	-1.35005	-0.78626	9.18032	-13.03818	9.60894	-2.75519	0.0012

TABLE I: Estimated energy per hole in the thermodynamic limit. The functional form of the fit is a 5th order polynomial $E^h(\delta) = \sum_{i=0}^5 a_i \delta^i$ determined by the largest cluster data in the region $\delta_c < \delta \leq 1$. The rightmost column represents the maximum error of the fit for $\delta \times E_h(\delta)$ (the energy per site referenced to the undoped case). E_{min}^h represents the estimated minimum energy per hole for $\delta \rightarrow 0$. Number(s) between brackets indicate error bars in the last digit(s).

Conclusions: We have introduced a technique for controlling finite size effects in an efficient way, an approach

particularly suited for the AFQMC method. In this way a strong numerical evidence is given that phase separation

is robust at small dopings and U/t values. With this approach it is possible to study other possible phases^{18–20}, with a better control of finite size effects at incommensurate dopings and weak couplings, as well as it is possible to export the method to other techniques, that may have problem of convergence to the thermodynamic limit especially at weak couplings. Indeed we have preliminary verified that, by choosing boundary conditions that break the symmetry of the lattice (e.g. cylindrical), much better results (i.e. much closer to the thermodynamic limit) can be obtained by correcting the energy levels of the $U = 0$ Hamiltonian according to the proposed method. Finally we want to remark that the method can be easily extended to realistic calculations that do not explicitly require a local Hamiltonian^{21,22} as in AFQMC. This can be achieved by considering as an input for the correlated

calculation the band-resolved DOS obtained with an uncorrelated Hamiltonian, such as the Khon-Sham one in Density Functional Theory. The same technique as above can be used to reduce finite size effects by preserving charge neutrality even in presence of the Coulomb long range interaction, a property that is difficult to fulfill with TABC, if we require that the non interacting limit should remain exact with a finite supercell calculation.

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This supplementary material contains energies of the Hubbard model with the AFQMC method described in the paper for various cluster sizes with periodic boundary conditions rotated by 45 degrees. These square lattices have an even number of sites $L = 2n^2$ where n is an odd (even) integer with PBC (APBC), and fulfill all rotation symmetries of the infinite lattice. In all the tables error bars are between brackets with usual conventions. In all the forthcoming results the guiding function is defined by means of the ground state ψ_{MF} of the following mean field Hamiltonian:

$$H_{MF} = \bar{K} - \mu_0 N + \left[\Delta_{AF} \sum_R (-1)^{x+y} c_{R,\uparrow}^\dagger c_{R,\downarrow} + \Delta_{BCS}^{x^2-y^2} \sum_k (\cos k_x - \cos k_y) c_{k,\uparrow}^\dagger c_{-k,\downarrow}^\dagger + \text{h.c.} \right] \quad (1)$$

where \bar{K} is the modified kinetic energy with MBC and $\mu_0 \neq 0$ is used when $\Delta_{BCS}^{x^2-y^2} \neq 0$ as the non interacting chemical potential value, namely at the middle of the non interacting highest energy occupied level $\bar{\epsilon}_{i_F+1}$ and lowest energy unoccupied level $\bar{\epsilon}_{i_F}$, $\mu_0 = \frac{\bar{\epsilon}_{i_F+1} + \bar{\epsilon}_{i_F}}{2}$, $N = \sum_{k,\sigma} c_{k,\sigma}^\dagger c_{k,\sigma}$ being the total number of particle operator that is not modified within the MBC approach. $R = (x, y)$ is a lattice point belonging to this lattice, namely $R = (x, y)$ is equivalent to $(x \pm n, y + n)$.

The results for the hole energy for $U/t = 1, 2, 3, 4$ are summarized in Fig.(1). The Trotter discretization time is chosen to have a positive systematic error (the values reported are variational upper bound of the energy) in the energy per site within $2 \times 10^{-4}t$, namely $\Delta t \times t = \frac{1}{4}, \frac{1}{6}, \frac{1}{8}, \frac{1}{10}$ for $U/t = 1, 2, 3, 4$, respectively. This error, being systematic and similar for nearby dopings, is expected to cancel out for the computation of the hole energy at small dopings, that, in this case, is affected only by the statistical error. Notice that, thanks to the symmetrized expression of the short time propagator:

$$\exp(-\Delta\tau H) \simeq \exp\left(-\frac{\Delta\tau}{2} K\right) \exp(-\Delta\tau V) \exp\left(-\frac{\Delta\tau}{2} K\right) \quad (2)$$

the Trotter error in the energy becomes almost negligible if measured after long imaginary time projection, as it is scaling as $(\Delta\tau)^4$,¹ and is also variational in the "Var" case mentioned in the paper because it corresponds to an energy expectation value of a given state.

For the smallest doping and largest clusters and $U/t > 2$ values, in order to have converged energies, it is necessary to optimize the trial function. Only at $U/t = 4$ we have found convenient to use a mean field Hamiltonian with a small d -wave superconducting order parameter. In general $\Delta_{BCS}^{x^2-y^2}$ and especially Δ_{AF} are useful in the small doping region.

¹ At leading order the approximate ground state wave function $|\psi_{\Delta\tau}^{GS}\rangle$ as a function of $\Delta\tau$ can be written as $|\psi_{\Delta\tau}^{GS}\rangle = |\psi^{GS}\rangle + \Delta\tau^2 |\psi'\rangle + O(\Delta\tau^3)$ where $|\psi'\rangle$ is orthogonal to the exact ground state $|\psi^{GS}\rangle$. Thus it is simple to show that the approximate ground state energy $E(\Delta\tau) = \frac{\langle \psi_{\Delta\tau}^{GS} | H | \psi_{\Delta\tau}^{GS} \rangle}{\langle \psi_{\Delta\tau}^{GS} | \psi_{\Delta\tau}^{GS} \rangle}$ does not contain the leading $O(\Delta\tau^2)$ order in the expansion, and that, with simple inspection, the first non zero contribution is vanishing as $\Delta\tau^4$

L	N_h	$U/t = 1$	$U/t = 2$	$U/t = 3$	$U/t = 4$
18	0	-1.383984(25)	-1.174357(42)	-.995837(80)	-.851727(22)
18	8	-1.316280(18)	-1.258224(50)	-1.210676(57)	-1.171736(17)
18	16	-.404113(4)	-.402104(12)	-.400564(15)	-.399349(4)
32	0	-1.383759(19)	-1.173957(49)	-.996540(66)	-.851421(35)
32	8	-1.427314(18)	-1.315238(40)	-1.220670(61)	-1.141815(28)
32	24	-.802289(8)	-.791310(14)	-.782523(24)	-.775319(17)
50	0	-1.383931(9)	-1.175175(26)	-.999904(34)	-.856989(29)
50	8	-1.432718(9)	-1.289485(22)	-1.167422(25)	-1.065190(50)
50	24	-1.279282(8)	-1.228975(19)	-1.187942(20)	-1.154477(15)
50	40	-.671976(3)	-.665129(9)	-.659723(10)	-.655354(6)
50	48	-.154689(1)	-.154454(2)	-.154276(2)	-.154139(2)
72	0	-	-	-1.000386(41)	-.857926(40)
72	8	-	-	-1.123689(54)	-1.007007(30)
72	24	-	-	-1.239880(23)	-1.180751(37)
72	40	-	-	-1.116184(17)	-1.092080(30)
72	48	-	-	-.953056(13)	-.939974(24)
72	64	-	-	-.400496(6)	-.399212(10)
98	0	-1.383884(17)	-1.175669(28)	-1.001029(53)	-.859353(19)
98	8	-1.417291(113)	-1.242952(157)	-1.093107(165)	-.968388(37)
98	24	-1.428730(86)	-1.315649(123)	-1.220505(82)	-1.141423(43)
98	40	-1.348419(86)	-1.281963(95)	-1.227174(45)	-1.182168(17)
98	48	-1.268210(58)	-1.219844(107)	-1.180124(43)	-1.147767(19)
98	56	-1.158019(59)	-1.124638(87)	-1.097401(41)	-1.075118(17)
98	72	-.839414(50)	-.826997(55)	-.817283(28)	-.809193(10)
98	80	-.626355(26)	-.620616(36)	-.616013(20)	-.612351(8)
98	88	-.374069(17)	-.372394(30)	-.371059(12)	-.370032(4)
98	96	-.080244(4)	-.080195(5)	-.080132(7)	-.080112(1)
128	0	-	-	-1.001331(40)	-
128	8	-	-	-1.071665(50)	-
162	0	-1.383989(68)	-1.175761(25)	-1.001315(46)	-.859880(39)
162	8	-1.405966(77)	-1.217640(156)	-1.056538(36)	-.926461(650)
162	24	-1.431606(55)	-1.284265(104)	-1.158330(69)	-1.052891(110)
162	40	-1.428448(56)	-1.316032(108)	-1.221628(340)	-
162	56	-1.391377(56)	-1.308639(113)	-1.240138(69)	-
162	64	-1.358795(55)	-1.289391(99)	-1.231708(36)	-
162	72	-1.316351(55)	-1.258192(80)	-1.210626(37)	-
162	88	-1.199681(41)	-1.161410(84)	-1.130263(28)	-
162	104	-1.037246(42)	-1.014225(82)	-.995547(21)	-
162	112	-.937604(37)	-.920560(60)	-.907076(19)	-
162	120	-.824934(29)	-.813331(64)	-.803772(14)	-
162	136	-.558768(20)	-.554421(39)	-.551001(11)	-
162	144	-.404113(14)	-.402095(22)	-.400539(9)	-
162	152	-.234318(10)	-.233719(20)	-.233277(7)	-
162	160	-.048875(2)	-.048852(4)	-.048838(1)	-
242	0	-1.383905(64)	-1.175775(63)	-1.001435(26)	-.860127(38)
242	8	-1.399151(64)	-1.203729(159)	-	-
242	24	-1.422228(55)	-1.255013(59)	-	-
242	40	-1.433352(67)	-1.292197(45)	-	-
242	56	-1.430992(59)	-1.313451(30)	-	-
242	72	-1.413774(59)	-1.317353(24)	-	-
242	80	-1.399206(48)	-1.312518(24)	-	-
242	88	-1.380472(62)	-1.302740(23)	-	-
242	104	-1.330079(51)	-1.268556(21)	-	-
242	120	-1.261094(49)	-1.213780(19)	-	-
242	136	-1.172439(51)	-1.137193(20)	-	-
242	144	-1.120353(43)	-1.090458(17)	-	-
242	152	-1.062959(31)	-1.037906(15)	-	-
242	168	-.931407(31)	-.914761(16)	-	-
242	184	-.776579(27)	-.766544(11)	-	-
242	192	-.690070(20)	-.682683(10)	-	-
242	200	-.597216(21)	-.592090(8)	-	-
242	216	-.392008(14)	-.390109(5)	-	-
242	224	-.279298(10)	-.278419(4)	-	-
242	232	-.159624(6)	-.159371(2)	-	-
242	240	-.032829(2)	-.032820(0)	-	-
1058	0	-1.383674(124)	-1.175469(92)	-1.001412(52)	-
1058	8	-1.387331(148)	-1.181826(91)	-1.009482(123)	-
1058	24	-1.394317(55)	-1.194489(118)	-1.026282(233)	-
1058	40	-1.400945(57)	-1.207317(101)	-	-
1058	56	-1.406985(56)	-1.220974(62)	-	-

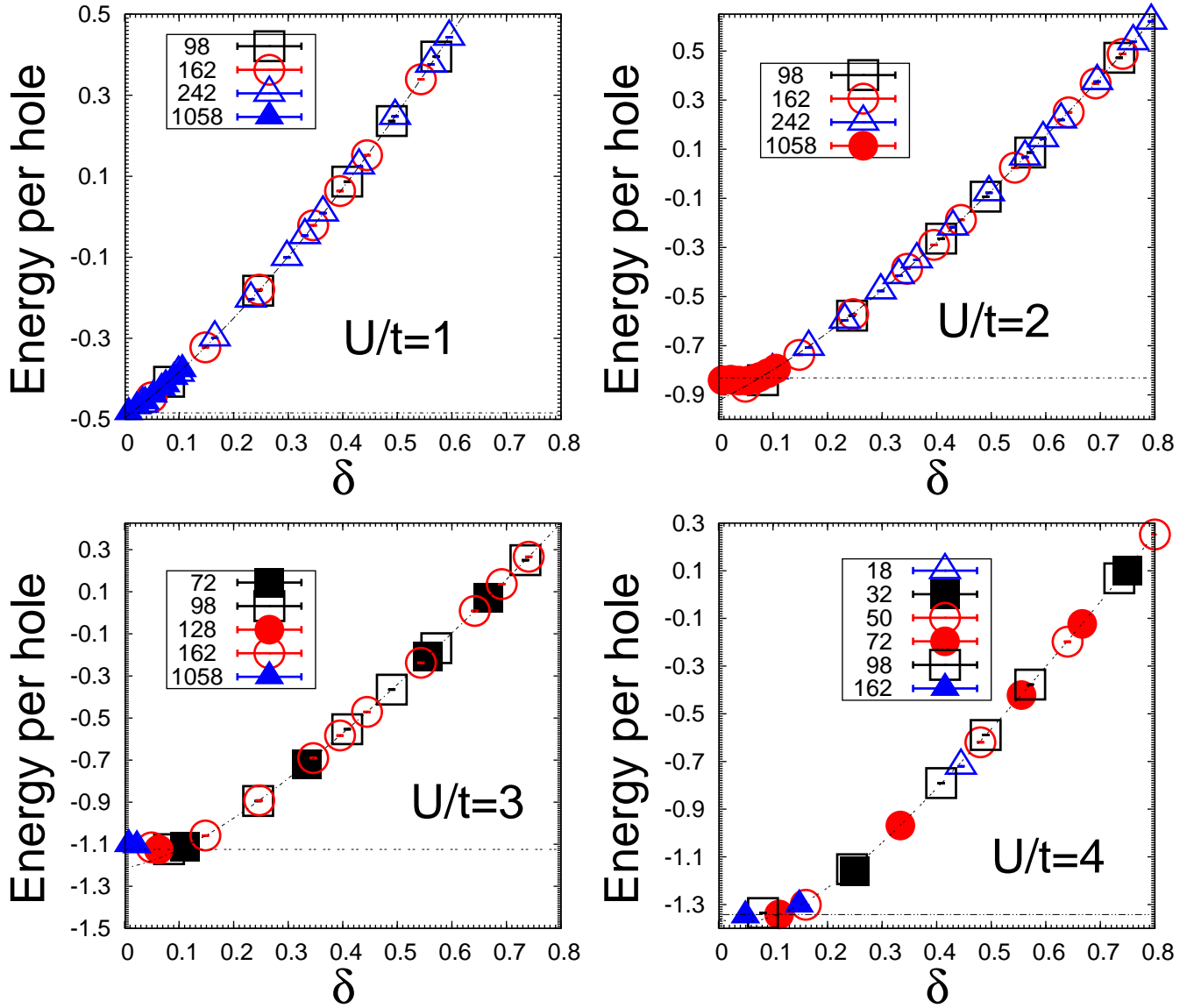


FIG. 1: Energy per hole for various U/t and cluster sizes. The curved lines are fit to the data with 5th order polynomials (see main text). The horizontal lines are the lowest hole energies estimated at the smallest available δ on the largest clusters.